060308 Quiz 8 Morphology of Complex Materials

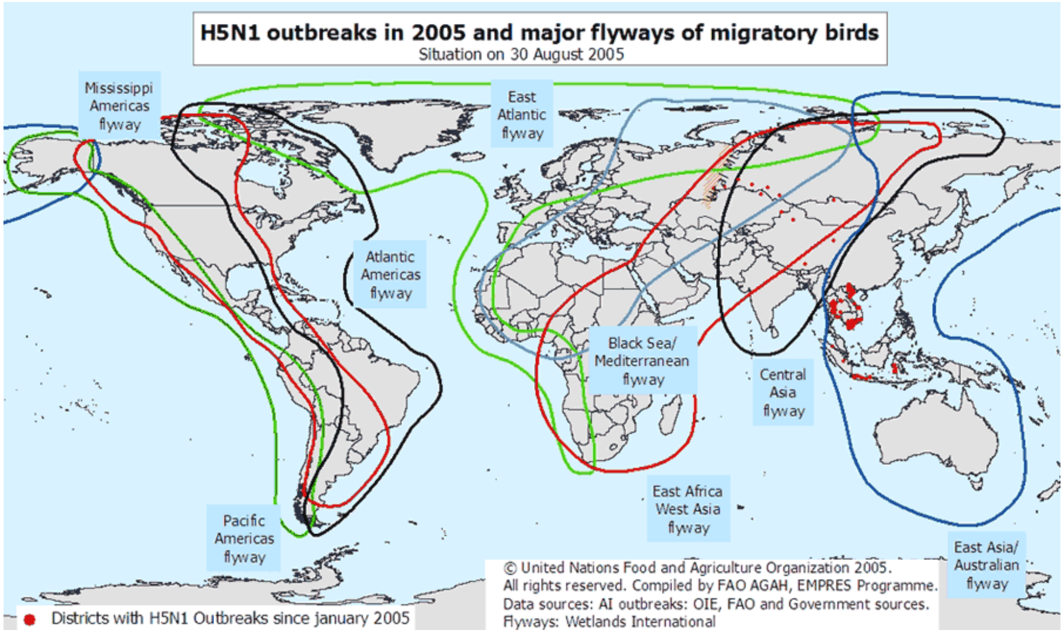

Figure 1. Migratory flight paths.

Above is a map of migration routes for birds which can carry the dreaded bird flu pandemic. Public Health scientists worry most about locations in central China since they connect with most of the world in a single year. The human population is like a supersaturated phase which can be nucleated (infected) at random locations along these flyways almost instantaneously (spontaneous nucleation). The World Health Organization has information concerning the fraction of the overall population infected as a function of time from hospital records, ϕ_{inf}. By constant monitoring it is possible to know the exact time of mutation of a human virulent strain (t_0 for "*nucleation*").

1) Assuming constant infection rate in terms of distance per time, dr/dt, from a "*nucleation*" site and complete infection of a region after an infection front passes through, derive an expression for ϕ_{inf} as a function of time that relies on the geometry of spreading by:
   a) Writing the Poisson distribution and explain the use of this distribution for this situation.
   b) Writing an expression for the average number of infection fronts that have passed through a random point at time t, <F> if infection spreads in 2d rings at a rate of dr/dt.
   c) Using the expression from "b" to write an expression for the expected behavior of ϕ_{inf} with time.
   d) If it is observed that ϕ_{inf} follows (1 - exp(-kt)) where t is time and k is a constant, what can be said about the transmission of the flu (perhaps along trade routes)? What is *k*?
   e) Could sporatic nucleation explain the behavior seen in part "d"? How or Why?

2) We discussed the hierarchy of aggregate materials such as the cosmic dust aggregate shown below, fig. 2 a.
   a) Explain the hierarchy of an aggregate structure and
   b) Compare it with the hierarchy of a linear polymer chain in solution.

c) What are the differences between these two structures?

d) If a chain aggregate (like the cosmic dust) is stretched would it behave in the same way as a polymer chain in thermal equilibrium? Explain your answer.

e) Explain the terms minimum path, p, minimum dimension d_{min}, connectivity ratio c and mass fractal dimension d_f.

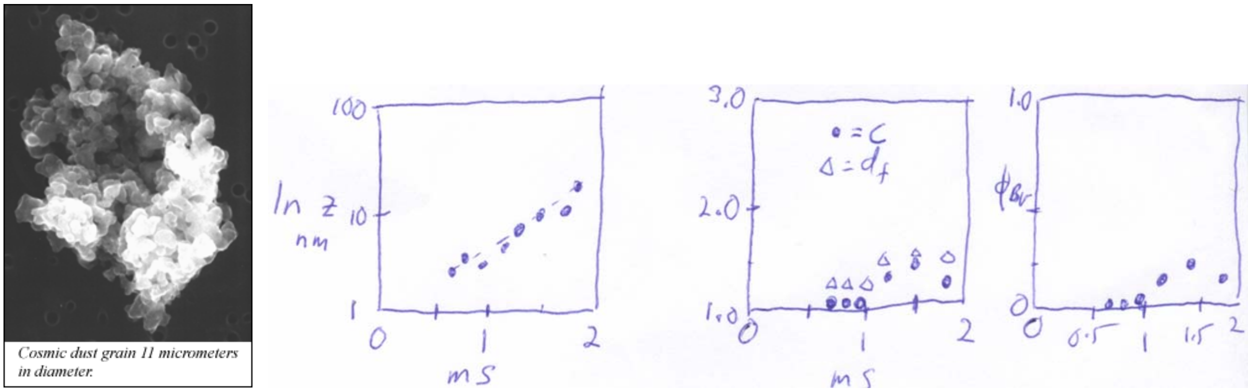

Figure 2. a) From NASA, b), c) and d) sketch of behavior of nanoparticle growth in spray flame.

3) The plot above (2b,c,d) shows the aggregation rate, aggregate size, z, versus t for alumina aggregates growing in a spray flame. The process occurs at about 1500 K and aggregation is complete in 1 ms.

a) If it is assumed that the fraction aggregate, ϕ_{Agg} is proportional to the average z (first figure, z is the mean number of primary particles in an aggregate), and that the behavior in the first plot is linear, what is the geometry of growth and type of nucleation for these aggregates based on the Avrami equation (that is if $\ln\phi_{Agg}$ is linear in t). Explain your answer.

b) Does the value of c in the third figure support your idea? Explain.

c) Does the value of d_f support your idea? Explain.

d) The branch fraction, ϕ_{Br}, in Figure 2d is defined by $\phi_{Br} = (z-p)/z$. Explain this function using a sketch of an aggregate.

e) What is ϕ_{Br} for a 6 arm star polymer?

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1a) $p(F) = \dfrac{\langle F\rangle^{F}\ \exp(-\langle F\rangle)}{F!}$

The Poisson distribution gives the probability that a low likelihood event will occur F times if the average number of times that it occurs is <F>. For our case we are interested in p(F=0) given by exp-<F>. since the total infected fraction is 1 - p(F=0).

b) <F> = N π (t dr/dt)^2, where N is the number of nucleation sites per area.

c) ϕ_{inf} = 1 - exp(Nπ(dr/dt)^{2}t^2)

d) If ϕ_{inf} is linear in time then nucleation is spontaneous and growth is linear. For linear growth k is N(dr/dt) where N is the number of nuclei per length in the system. Linear growth might occur if growth of infection occurred along highways or trade routes in a straight line rather than in 2d space.

e) Sporatic nucleation could not explain the behavior in part "d" since the lowest time power is 2 for sporatic nucleation.

2) a) b)

<u>Aggregate</u>	<u>Polymer</u>
Primary particle	Persistence length
Size distribution	(Helix)
Fractal structure	Chain scaling
Branch structure	
Agglomerates	

c) Polymer hierarchy is determined by thermodynamics while the aggregate structure is determined by kinetics. The persistence length does not display a distribution in size. Aggregates tend to have a high degree of branching due to the nature of the bonding event.

d) The polymer chain obeys rubber elasticity with the chain spring constant being proportional to 3kT/p, while the chain aggregate displays Hooken behavior.

e) p is the number of primary particles in a connected path through the aggregate that has the minimum length from one side to the other. The straight distance between the two sides is R. Then, $(R/l_p)^{dmin}$ = p, $(R/l_p)^{df}$ = z, and z = p^c.

3) a) If lnϕ_{Agg} is linear in t then the Avrami power is 1 and growth is 1-d so the initial aggregates should be linear structures with c = 1 and ϕ_{Br} = 0.

b) The value of c is close to 1 initially but later it increases to 1.2. This means that the structures become more branched later.

c) The value of d_f is 1.2 at the start of growth and approaches 1.5 at the end so it is a convoluted path structure. The growth is still linear.

d) z is the total number of primary particles and p is the number of primary particles in the minimum path. ϕ_{Br} represents the mass in branches divided by the total mass. This is typically on the order of 0.8 or higher for a branched aggregate. Here ϕ_{Br} is on the order of 0.3 so these are weakly branched structures.

e) For a 6 arm star two arms make p and the total mass is z = 3p so z-p = 2p and ϕ_{Br} = 0.67